

DEVELOPMENT OF A FORMALISM OF DISCRETE ELEMENT METHOD TO STUDY MECHANICAL RESPONSE OF GEOLOGICAL MATERIALS AND MEDIA AT DIFFERENT SCALES

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Summary. A general approach to realization of models of elasticity, plasticity and fracture of heterogeneous materials within the framework of particle-based discrete element method is proposed in the paper. The approach is based on constructing many-body forces of particle interaction, which provide response of particle ensemble correctly conforming to the response (including elastic-plastic behavior and fracture) of simulated solids. For correct modeling of inelastic deformation and failure of geological materials and media at "high" structural scales (relative to the scale of grains) an implementation of dilatational Nikolaevsky's model of plasticity of rocks within the framework of mathematical formalism of discrete element method is proposed. Perspectives of multiscale modeling of geological materials from grain-related scale up to macroscopic scale within the same numerical technique (DEM) are discussed.

1 INTRODUCTION

At present time numerical particle-based methods, belonging to the group of discrete element methods (DEM), are widely used for the study of deformation and fracture of weakly bonded and loose media as well as of brittle materials (including rocks). The main feature and advantage of DEM is an "inherent ability" to directly simulate fracture (including multiple fracture) and mass mixing phenomena. This determined primary application of this numerical technique to study the features and mechanisms of material response at the "microscale", i.e. at the scale of structural elements of considered system (grains of sand or rock, powder particles, blocks in zones of localized intensive fragmentation of massifs and so on). Such studies are crucial for understanding the basic (elementary) mechanisms of inelastic deformation and failure in block-structured media as well as for the construction of rheological models of complex media [1,2]. Such rheological models can be used for theoretical study of the behavior of hierarchically organized geological media at high structural scales (that is, such models serve as a basis of multiscale modeling).

One of the most important fundamental problems in DEM, as well as in other methods of particles, is determination of the form of potential/force of particle interaction. The form and

parameters of forces of particle-particle interaction in many respects determine the “integral” response of the ensemble, including its compliance with the response of the simulated medium. It has to be noted that microscale description of loose or consolidated brittle materials (including rocks) within the DEM is conventionally done with use of pair-wise models of element-element interaction (including pair-wise formulation of fracture criteria) [1,3]. Such simplification of element-element interaction strongly limits fields of application of DEM. In particular, application of pair-wise models of interaction between discrete elements to study loose material at macroscale often fails. Moreover, DEM-based description of consolidated rocks at meso- and macroscopical scales with use of pair-wise interaction potentials is not capable to take into account damage generation phenomena at spatial scales lower than discrete element size. As a consequence rock and soil behavior at “high” spatial/structural scales (with respect to grain-related scale) is conventionally described with use of numerical methods of continuum mechanics (FEM, FDM and so on). The main advantage of these methods is a capability to implement various (including multiparametric) rheological models.

Research conducted by the authors has shown that an adequate description of deformation and fracture of heterogeneous materials at different spatial scales is possible with the use of many-body potentials/forces of discrete element interaction. The authors propose an approach to building relationships for the central and tangential potential forces of particle interaction. The structure of the expression for interaction force is analogous to the structure of interatomic potentials in the embedded-atom model. This approach is implemented in the framework of the movable cellular automaton method (MCA), which is a new and intensively developed representative of the group of computational methods of particles [4,5]. The paper demonstrates the main theses of the developed approach and methods of implementation of various rheological models of heterogeneous materials. In particular, implementation of Nikolaevsky’s model of plasticity (the generalized Drucker-Prager plasticity model with Mises-Schleicher criterion and non-associated flow law) within the DEM is proposed for an adequate description of inelastic deformation of hierarchically organized geological medium. A way to implement multiparametric fracture criteria within the DEM for the correct modeling of the fracture in complex geological media at “high” structural scales (relative to the spatial scale of the elementary structural elements) is proposed as well.

2 GENERAL FORMALISM OF MANY-BODY INTERACTION

Proposed general form of many-body forces of interaction between discrete elements is borrowed from the form of interatomic forces calculated on the basis of embedded-atom method. In the framework of embedded-atom model the general expression for potential energy of atom i contains a pair interaction potential ϕ as a function of distance r_{ij} between atoms i and j and a “density-dependent” embedding function F (here it depends on electron charge density $\bar{\rho}_i$):

$$E_i(R) = \sum_{j \neq i} \phi(r_{ij}) + \sum_i F(\bar{\rho}_i) \quad (1)$$

where $\bar{\rho}_i = \sum_{j \neq i} \rho_j(r_{ij})$ is a sum of contributions of neighbors j to local value of density at the location of atom i . By analogy with this expression the following general form of notation of

the expression for the force \vec{F}_i acting on discrete element i from surroundings is proposed:

$$m_i \frac{d^2 \vec{R}_i}{dt^2} = \vec{F}_i = \sum_{j=1}^{N_i} \vec{F}_{pair}^{ij} + \vec{F}_\Omega^i \quad (2)$$

This force is written as a superposition of pair-wise constituents \vec{F}_{pair}^{ij} depending on spatial position/displacement of element i with respect to nearest neighbor j and of volume-dependent constituent \vec{F}_Ω^i connected with combined influence of nearest surroundings of the element.

When simulating locally isotropic materials/media the volume-dependent contribution \vec{F}_Ω^i can be expressed in terms of pressure P_i in the volume of discrete element i as follows [5]:

$$\vec{F}_\Omega^i = -A_i \sum_{j=1}^{N_i} P_i S_{ij} \vec{n}_{ij} \quad (3)$$

where S_{ij} is square of area of interaction (contact) of elements i and j , \vec{n}_{ij} is a unit vector directed along the line between mass centres of considered elements, A_i is a material parameter for the element i (in general case each element simulates a material fragment with unique phase or chemical composition and is characterized by a unique value of material parameter A).

In such a formulation the right part of the expression (2) can be reduced to the sum of forces of interaction in pairs of elements and divided into central (\vec{F}_n^{ij}) and tangential (\vec{F}_t^{ij}) constituents:

$$\vec{F}_i = \sum_{j=1}^{N_i} (\vec{F}_{pair}^{ij} - A_i P_i S_{ij} \vec{n}_{ij}) = \sum_{j=1}^{N_i} [F_{pair,n}^{ij}(h_{ij}) - A_i P_i S_{ij}] \vec{n}_{ij} + F_{pair,t}^{ij}(l_{is}^{shear}) \vec{t}_{ij} = \sum_{j=1}^{N_i} (\vec{F}_n^{ij} + \vec{F}_t^{ij}) \quad (4)$$

where $F_{pair,n}^{ij}$ and $F_{pair,t}^{ij}$ are central and tangential components of pair-wise interaction force that depend on the values of element-element overlap h_{ij} and relative shear displacement l_{ij}^{shear} (l_{ij}^{shear} is calculated taking into account rotations of both elements of the pair [1,4]), \vec{t}_{ij} is a unit vector which is oriented perpendicular to the line joining the centers of mass of elements i and j . For conveniences hereinafter interaction forces will be considered in specific units (σ_{ij} and τ_{ij}) obtained by dividing the total values (\vec{F}_n^{ij} and \vec{F}_t^{ij} correspondingly) by S_{ij} . In terms of specific interaction forces σ_{ij} and τ_{ij} the expression (4) takes the following form:

$$\begin{cases} \sigma_{ij} = \sigma_{ij}^{pair}(h_{ij}) - A_i P_i \\ \tau_{ij} = \tau_{ij}^{pair}(l_{ij}^{shear}) \end{cases} \quad (5)$$

where σ_{ij}^{pair} and τ_{ij}^{pair} are pair-wise components of specific interaction forces. Specific forces σ_{ij} and τ_{ij} can be interpreted as forces of response of the element (or movable cellular automaton) i to the impact of the neighbour j . In general case interacting elements i and j has different material properties. Therefore reaction forces σ_{ij}^{pair} and τ_{ij}^{pair} depend not on the total values of pair overlap and shear displacement but on contributions of the element i to total

values of these spatial parameters. Hereinafter such contributions will be considered in normalized units:

$$\begin{cases} \Delta h_{ij} = \Delta q_{ij} + \Delta q_{ji} = \Delta \varepsilon_{i(j)} d_i / 2 + \Delta \varepsilon_{j(i)} d_j / 2 \\ \Delta l_{ij}^{shear} = \Delta \gamma_{i(j)} q_{ij} + \Delta \gamma_{j(i)} q_{ji} \end{cases} \quad (6)$$

where symbol Δ hereinafter indicates increment of corresponding parameter during one time step Δt , q_{ij} and q_{ji} are the distances from mass centers of elements i and j to the center of area of interaction ($q_{ij} + q_{ji} = r_{ij}$; r_{ij} is the distance between mass centers of elements), d is size of element, $\varepsilon_{i(j)}$ and $\varepsilon_{j(i)}$ are central strains of discrete elements i and j in the pair, $\gamma_{i(j)}$ and $\gamma_{j(i)}$ are shear angles of discrete elements i and j in the pair (in the general case $\varepsilon_{i(j)} \neq \varepsilon_{j(i)}$ and $\gamma_{i(j)} \neq \gamma_{j(i)}$). The law of distribution of total values h_{ij} and l_{ij}^{shear} between discrete elements i and j is inseparably linked with concrete form of pair wise constituents σ_{ij}^{pair} and τ_{ij}^{pair} and can be derived from the necessary requirement of satisfaction of Newton's third law for interacting pairs of discrete elements ($\sigma_{ij} = \sigma_{ji}$ and $\tau_{ij} = \tau_{ji}$):

$$\begin{cases} \sigma_{ij} = \sigma_{ij}^{pair}(\varepsilon_{i(j)}) - A_i P_i \equiv \sigma_{ji} = \sigma_{ji}^{pair}(\varepsilon_{j(i)}) - A_j P_j \\ \tau_{ij} = \tau_{ij}^{pair}(\gamma_{i(j)}) \equiv \tau_{ji} = \tau_{ji}^{pair}(\gamma_{j(i)}) \end{cases} \quad (7)$$

Equations (6)-(7) provides the basis for calculation of contributions of elements i and j ($\varepsilon_{i(j)}$ and $\varepsilon_{j(i)}$, $\gamma_{i(j)}$ and $\gamma_{j(i)}$) to the total values of pair overlap and relative shear displacement as well as for calculation of the forces \vec{F}_n^{ij} and \vec{F}_t^{ij} of pair interaction.

It is seen from (7) that an important problem in building many-particle interaction is definition of local value of pressure (P_i) in the volume of discrete element. Authors propose to use an approach to calculation of pressure P_i (or, what is the same – of mean stress) in the volume of the element i that is based on the computation of components of average stress tensor in the volume of the element [1]. In terms of specific central (σ_{ij}) and tangential (τ_{ij}) interaction forces the component $\bar{\sigma}_{\alpha\beta}^i$ of average stress tensor in the volume of element i can be written as follows [1,6]:

$$\bar{\sigma}_{\alpha\beta}^i = \frac{1}{\Omega_i} \sum_{j=1}^{N_i} S_{ij} q_{ij} (\vec{n}_{ij})_{\alpha} \left[\sigma_{ij} (\vec{n}_{ij})_{\beta} + \tau_{ij} (\vec{t}_{ij})_{\beta} \right] \quad (8)$$

where $\alpha, \beta = x, y, z$ (XYZ is a laboratory system of coordinates), Ω_i is a current value of the volume of element i , $(\vec{n}_{ij})_{\alpha}$ and $(\vec{t}_{ij})_{\alpha}$ are projections of unit-normal and unit-tangential vectors onto the X-axis of lab coordinates.

Calculated in this way the stress tensor components can be used to determine the pressure in the volume of discrete element as well as other tensor invariants, for example stress intensity:

$$P_i = -\bar{\sigma}_{mean}^i = -\frac{\bar{\sigma}_{xx}^i + \bar{\sigma}_{yy}^i + \bar{\sigma}_{zz}^i}{3} \quad (9)$$

$$\bar{\sigma}_{\text{int}}^i = \frac{1}{\sqrt{2}} \sqrt{\left(\bar{\sigma}_{xx}^i - \bar{\sigma}_{yy}^i\right)^2 + \left(\bar{\sigma}_{yy}^i - \bar{\sigma}_{zz}^i\right)^2 + \left(\bar{\sigma}_{zz}^i - \bar{\sigma}_{xx}^i\right)^2 + 6\left[\left(\bar{\sigma}_{xy}^i\right)^2 + \left(\bar{\sigma}_{yz}^i\right)^2 + \left(\bar{\sigma}_{xz}^i\right)^2\right]}$$

The main advantage of the developed approach to building expressions for forces of interaction of discrete elements (or movable cellular automata) is a possibility to implement various rheological models of heterogeneous medium within the formalism of DEM [6].

In particular, to adequately describe response of hierarchically organized geological medium at various structural/spatial scales with regard to the contributions of “embedded” structural scales of lower ranks, the two-parametric rheological model with non-associated plastic flow law and Drucker-Prager yield criterion (Nikolaevsky’s model) is widely used. Below is an implementation of this model within the framework of discrete element approach.

3 DISCRETE ELEMENT INTERACTION FOR MODELING ELASTIC-PLASTIC MEDIUM

3.1 Linearly elastic medium

Response of isotropic material, which is under the stress state inside the limiting surface (in stress space), is conventionally described on the basis of generalized Hooke’s law. The following notation of this law will be used hereinafter:

$$\begin{cases} \sigma_{\alpha\alpha} = 2G\varepsilon_{\alpha\alpha} + (1 - 2G/K)\sigma_{\text{mean}} \\ \tau_{\alpha\beta} = G\gamma_{\alpha\beta} \end{cases} \quad (10)$$

where $\alpha, \beta = x, y, z$; $\sigma_{\alpha\alpha}$ and $\varepsilon_{\alpha\alpha}$ are diagonal components of stress and strain tensors; $\tau_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ are off-diagonal components; $\sigma_{\text{mean}} = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$ is mean stress; K is bulk modulus; G is shear modulus.

It can be seen that the form and the matter of expressions (10) for diagonal and off-diagonal stress tensor components are analogous to expressions (5) and (7) describing normal and tangential interaction of discrete elements. This leads to the simple idea to write down expressions for force response of element i to the impact of the neighbor j by means of direct reformulation of Hooke’s law relationships:

$$\begin{cases} \sigma_{ij} = 2G_i\varepsilon_{i(j)} + \left(1 - 2G_i/K_i\right)\bar{\sigma}_{\text{mean}}^i \\ \tau_{ij} = 2G_i\gamma_{i(j)} \end{cases} \quad (11)$$

where G_i and K_i are shear and bulk elastic moduli of material filling the element i , mean stress $\bar{\sigma}_{\text{mean}}^i$ is calculated using (9). Note that double shear modulus ($2G_i$) is used in the second expression of (11) instead of G in (10). This feature is concerned with the fact that relative tangential displacement of discrete elements leads to their rotations. Initiated rotation of the elements decreases twice the value of relative shear displacement in interacting pairs.

Proposed relationships (11) for forces of the element response to the impact of the neighbor j provide implementation of the Hooke’s law for components $\bar{\sigma}_{\alpha\beta}^i$ of average stress tensor in the volume of element i . This can be shown by substituting expressions (11) for respond force in (8). Detail description can be found in the paper [6].

Relationships (11) make it possible to calculate central and tangential interaction of discrete elements, whose ensemble simulates isotropic elastic medium. Substituting (11) into (7) and taking into account (6) it is easy to obtain the system of expressions to calculate specific interaction forces in the pair i - j :

$$\begin{cases} \sigma_{ij}^{cur} = \sigma_{ij}^{pre} + \Delta\sigma_{ij} = \sigma_{ij}^{pre} + 2G_i\Delta\varepsilon_{i(j)} + \left(1 - \frac{2G_i}{K_i}\right)\Delta\bar{\sigma}_{mean}^i = \\ = \sigma_{ji}^{cur} = \sigma_{ji}^{pre} + \Delta\sigma_{ji} = \sigma_{ji}^{pre} + 2G_j\Delta\varepsilon_{j(i)} + \left(1 - \frac{2G_j}{K_j}\right)\Delta\bar{\sigma}_{mean}^j \\ \Delta h_{ij} = \Delta\varepsilon_{i(j)} \frac{d_i}{2} + \Delta\varepsilon_{j(i)} \frac{d_j}{2} \\ \begin{cases} \tau_{ij}^{cur} = \tau_{ij}^{pre} + \Delta\tau_{ij} = \tau_{ij}^{pre} + 2G_i\Delta\gamma_{i(j)} = \tau_{ji}^{cur} = \tau_{ji}^{pre} + \Delta\tau_{ji} = \tau_{ji}^{pre} + 2G_j\Delta\gamma_{j(i)} \\ \Delta l_{shear}^{ij} = \Delta\gamma_{i(j)} \frac{d_i}{2} + \Delta\gamma_{j(i)} \frac{d_j}{2} \end{cases} \end{cases} \quad (12)$$

Here, relations for calculating the central and tangential interaction forces are written in incremental fashion (in hypoelastic form); “*cur*” and “*pre*” upper indexes mark values of specific reaction forces at the current step of integrating the equations of motion of discrete elements (or cellular automata); mean stress increments $\Delta\bar{\sigma}_{mean}^i$ and $\Delta\bar{\sigma}_{mean}^j$ are taken from previous time step or determined with use of predictor-corrector modification of a numerical scheme. Equations (12) are first solved for strain increments $\Delta\varepsilon_{i(j)}$, $\Delta\varepsilon_{j(i)}$, $\Delta\gamma_{i(j)}$ and $\Delta\gamma_{j(i)}$. Found values of strain increments are then substituted to calculate current values of specific forces σ_{ij} and τ_{ij} .

Testing of the proposed model of element interaction by the example of elastic wave propagation showed that ensemble of discrete elements, which interact according to (12), demonstrates a “macroscopically” isotropic response, even with the regular packing of elements of the same size. Note that achieving isotropic response of regularly packed elements is a fundamental problem in conventional models of DEM that use approximation of two-particle interaction.

3.2 Elastic-plastic medium (Nikolaevsky’s model of plastic flow)

An important advantage of the proposed approach to building many-body interaction of discrete elements is a capability to realize various models of elasticity and plasticity within the framework of DEM (or MCA). In particular, non-associated plastic flow theory (namely, the generalized Drucker-Prager model with non-associated flow law within the limits of Nikolaevsky’s model) was implemented within DEM to simulate nonelastic mechanical response of brittle materials (including rock) at the mesoscopic or macroscopic structural scale. When constructing models of plasticity of geomaterials, it is necessary to take into account features of the mechanisms of relaxation of internal stresses. In contrast to metals and alloys, these mechanisms are associated with the formation and development of damages (cracks) of different ranks rather than with the movement of lattice defects. Under the simulation of geomaterials by ensemble of discrete elements the damages with a size comparable to or greater than the size of discrete element can be modeled directly through

breaking the bonds between linked (bonded) elements. The study of the dynamics of accumulation of such damages and their influence on the integrated response of the ensemble can be carried out in the framework of conventional models of linear-elastic interaction of discrete elements. At the same time, damages of smaller spatial scales must be taken into account implicitly by defining a model of plasticity (it is rather correct to speak about quasiplasticity) and selecting the appropriate structural form and parameters of yield criterion. In view of the features of functioning of the relaxation mechanisms in geomaterials (generation of damage is concerned with the formation of free surfaces and the emergence of a free volume) applied plasticity model must satisfy at least two conditions:

1. Plasticity criterion must take into account the effect of the local pressure (compressive hydrostatic pressure prevents the spatial diversity of the atomic planes and thus hinders generation/development of damages and cracks).

2. Plasticity model must take into account the effect of emergence of the free volume, that is to say, the possibility of inelastic volumetric deformation of the body.

One of such kind of models is a model of Nikolaevsky that adequately takes into account above described requirements. In the framework of this model the criterion of reaching the limit of elasticity is the condition of Mises-Schleicher [7,8]:

$$\Phi = \omega J_1 + \sqrt{J_2} = 3\omega\sigma_{mean} + \frac{\sigma_{int}}{\sqrt{3}} > Y, \quad (13)$$

where σ_{mean} and σ_{int} are mean stress and stress intensity, Y is the elastic limit of the material under shear loading, ω is proportional to the coefficient of internal friction. The main feature of Nikolaevsky's model is a postulated linear dependence of plastic volume strain rate on plastic shear strain rate:

$$\dot{\epsilon}_1^p = 2\Lambda\sqrt{\dot{\epsilon}_2^p} \quad (14)$$

The coefficient of proportionality Λ is called the coefficient (rate) of dilatancy.

Implementation of Nikolaevsky's model within the framework of DEM/MCA method was done with use of radial return algorithm of Wilkins [9] (note that before this algorithm was adopted to the DEM formalism to implement the plastic flow theory with von Mises yield criterion to simulate plastic deformation of metals [6]). The gist of this numerical scheme consists in solving the elastic problem in the current step of integration of the equations of motion of the particles and the subsequent scaling (returning) potential forces of particle interaction in compliance with the necessary requirements of Nikolaevsky's model for the values of local pressure and Mises-Schleicher criterion of plasticity [7].

Conventionally, radial returning of stresses is formulated in terms of the stress deviator \hat{D}_σ :

$$\hat{D}'_\sigma = \hat{D}_\sigma M, \quad (15)$$

where M is a coefficient of stress drop (stress scaling), \hat{D}_σ is a stress deviator after solution of elastic problem at the current time step, \hat{D}'_σ is a scaled stress deviator.

Being written in terms of stress, the algorithm of Wilkins for the applied model of plasticity can be presented in the following form:

$$\sigma'_{\alpha\beta} = (\sigma_{\alpha\beta} - \delta_{\alpha\beta} \sigma_{mean})M + \delta_{\alpha\beta} \sigma'_{mean}, \quad (16)$$

where $M = \sqrt{J'_2/J_2}$, $\delta_{\alpha\beta}$ is the Kronecker delta. Main requirements of the algorithm of Wilkins for the Nikolaevsky's model concern the values of "relaxed" (scaled) first and second invariants of stress tensor [7]:

$$\sqrt{J'_2} = \frac{\sigma'_{int}}{\sqrt{3}} = \sqrt{J_2} - \frac{G(\Phi - Y)}{K\Lambda\omega + G}, \quad (17)$$

$$J'_1 = 3\sigma'_{mean} = J_1 - \frac{K_i\Lambda_i(\Phi_i - Y_i)}{3K_i\Lambda_i\omega_i + G_i}.$$

The main problem in realization of the algorithm of Wilkins within the framework of DEM (or MCA) is formulation of correcting relations for element interaction forces that provide implementation of necessary conditions (17) for average stresses in the volume of discrete element. By analogy with the elastic problem the expressions for scaling specific central and tangential forces of response of the element i to the impact of the neighbor j can be derived by direct reformulation of relations (16) for average stresses. So, implementation of the above described algorithm within the framework of DEM formalism is as follows. At the current step of integration of the equations of motion the forces of interaction of elements (automata) are calculated in the elastic approximation according to (12). After that the components of average stress tensor ($\bar{\sigma}_{\alpha\beta}^i$) are computed for all discrete elements of the ensemble. Next, the condition (13) is checked for each element. In the case of fulfillment of this condition for the element/automaton i the correction (scaling) of its response forces $\sigma_{i(j)}^{cur}$ and $\tau_{i(j)}^{cur}$ in all pairs i - j is carried out as follows:

$$\begin{cases} \sigma'_{i(j)} = (\sigma_{i(j)}^{cur} - \bar{\sigma}_{mean}^i)M_i + (\bar{\sigma}_{mean}^i - N_i) \\ \tau'_{i(j)} = \tau_{i(j)}^{cur}M_i \end{cases}, \quad (18)$$

where $(\sigma'_{i(j)}, \tau'_{i(j)})$ are scaled values of specific response forces, $M_i = 1 - \frac{\sqrt{3}}{\bar{\sigma}_{int}^i} \frac{G_i(\Phi_i - Y_i)}{K_i\Lambda_i\omega_i + G_i}$ is a coefficient of scaling of stress deviator for the element i , $N_i = \frac{K_i\Lambda_i(\Phi_i - Y_i)}{3K_i\Lambda_i\omega_i + G_i}$ is a correction to the local (in the volume of element i) value of mean stress $\bar{\sigma}_{mean}^i$ calculated in the elastic approximation, Y_i , Λ_i and ω_i are instantaneous (current) values of model parameters for the material of element i . In the general case the model parameters in (18) are assumed to be functions of strain and strain rate.

By analogy with elastic problem substitution of (18) in expression (8) for average stress tensor automatically provides reduction of its components to yield surface for the element i . This gives possibility to correctly simulate quasiplastic behavior of brittle materials (including rocks) with multiscale internal structure by the ensemble of discrete elements.

Note that independent use of the expressions (18) for interacting elements i and j can lead to unequal values of response forces ($\sigma'_{ij} \neq \sigma'_{ji}$ and $\tau'_{ij} \neq \tau'_{ji}$) in the pair i - j . In view of the need

for implementation of Newton's third law the current values of element interaction forces in (4) are calculated on the basis of the following proportion:

$$\begin{cases} F_n^{ij} = S_{ij}\sigma_{ij} = S_{ij} \frac{\sigma'_{ij}q_{ji} + \sigma'_{ji}q_{ij}}{r_{ij}} \\ F_t^{ij} = S_{ij}\tau_{ij} = S_{ij} \frac{\tau'_{ij}q_{ji} + \tau'_{ji}q_{ij}}{r_{ij}} \end{cases} \quad (19)$$

In the framework of the applied two-parametric Nikolaevsky's model of plastic flow the material rheological properties of discrete elements are assigned by the dependencies $Y(\varepsilon_{ms}, \dot{\varepsilon}_{ms})$, $\omega(\varepsilon_{ms}, \dot{\varepsilon}_{ms})$ and $\Lambda(\varepsilon_{ms}, \dot{\varepsilon}_{ms})$. Here $\varepsilon_{ms} = \varepsilon_{mean} K\omega/G + \varepsilon_{int}/\sqrt{3}$ is a combination of the first two invariants of strain tensor (this parameter can be conventionally called "Mises-Schleicher deformation parameter"), $\dot{\varepsilon}_{ms}$ is a rate of change of this parameter. Note that the form of parameter ε_{ms} ensures the equality $\Phi/\varepsilon_{ms} = 3G$ within the region of elastic deformation (ε_{ms} can be considered as an analogue of equivalent strain in the conventional models of plasticity of metals with von Mises yield criterion). To construct the above mentioned dependencies of three listed model parameters, at least two types of mechanical tests (e.g. uniaxial compression and tension and/or pure shear) under various loading rates have to be held.

4 MODELING FRACTURE WITH DEM-BASED FORMALISM

One of the main advantages of particle-based methods in mechanics is the feasibility of direct simulation of fracture (including multiple fracture) of material through changing the state of a pair of particles ("linked" pair \rightarrow "unlinked" pair). The criterion for pair state switching is normally the ultimate value of interaction force or the ultimate value of relative displacement [1,3]. The developed approach to the description of interaction of discrete elements (or movable cellular automata) in the many-body approximation makes it possible to apply various multiparametric "force" fracture criteria (Drucker-Prager, Coulomb-Mohr, etc) as element-element bond fracture criteria.

In the framework of classical formalism of discrete elements pair bond breakage occurs on the surface of their interface (at the area of interaction of the pair, in other words, at the contact area). Therefore applied "force" failure criterion (for example, the criterion of Drucker-Prager) must be calculated at the area of interaction of elements using the local stress tensor components identified at this area [6]. In the local coordinate system $X'Y'$ of the interacting pair $i-j$ (Figure 1) components $\sigma_{y'y'}^{ij}$ and $\sigma_{x'y'}^{ij}$ of this local stress tensor are numerically equal to specific forces of central (σ_{ij}) and tangential (τ_{ij}) interaction of the elements (these forces are applied to the contact area S_{ij}):

$$\begin{cases} \sigma_{y'y'}^{ij} \equiv \sigma_{ij} \\ \sigma_{x'y'}^{ij} \equiv \tau_{ij} \end{cases} \quad (20a)$$

Other components ($\sigma_{x'x'}^{ij}$ and $\sigma_{z'z'}^{ij}$) of the local stress tensor can be determined on the basis of linear interpolation of corresponding values for elements i and j ($\bar{\sigma}_{x'x'}^i$ and $\bar{\sigma}_{x'x'}^j$, $\bar{\sigma}_{z'z'}^i$ and

$\bar{\sigma}_{z'z'}^j$) to the area of interaction:

$$\begin{cases} \sigma_{x'x'}^{ij} = \frac{\bar{\sigma}_{x'x'}^i q_{ji} + \bar{\sigma}_{x'x'}^j q_{ij}}{r_{ij}} \\ \sigma_{zz}^{ij} = \frac{\bar{\sigma}_{z'z'}^i q_{ji} + \bar{\sigma}_{z'z'}^j q_{ij}}{r_{ij}} \end{cases} \quad (20b)$$

where $\bar{\sigma}_{\alpha'\beta'}^i$ and $\bar{\sigma}_{\alpha'\beta'}^j$ are components of average stress tensor in the volume of elements i and j in the local coordinate system $X'Y'$ of the pair (these stresses result from transformation of average stresses $\bar{\sigma}_{\alpha\beta}^i$ and $\bar{\sigma}_{\alpha\beta}^j$ to local coordinates).

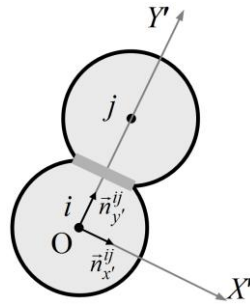


Figure 1: Instantaneous coordinate system associated with the current spatial orientation of the pair i - j .

Components $\sigma_{\alpha'\beta'}^{ij}$, thus defined, can be used to calculate necessary invariants of stress tensor which then can be used to calculate current value of applied criterion of pair fracture. Below the example of bond breaking condition for the pair i - j with use of Drucker-Prager criterion is shown:

$$\sigma_{\text{int}}^{ij} 0.5(a+1) + \sigma_{\text{mean}}^{ij} 1.5(a-1) > \sigma_c. \quad (21)$$

where σ_c is the corresponding threshold value for considered pair (value characterizing strength of cohesion/adhesion), $a = \sigma_c / \sigma_t$ is a ratio of compressive strength (σ_c) of the pair bond to tensile strength (σ_t), σ_{int}^{ij} and $\sigma_{\text{mean}}^{ij}$ are corresponding invariants of stress tensor $\sigma_{\alpha'\beta'}^{ij}$.

When using the explicit scheme of integration of motion equations the value of time step Δt is limited above by a quantity associated with the time of propagation of the sound through the volume of element. Normally time step is a quarter of this limit or less. In such a situation conventional model of breakage of bond in pair during one time step Δt is an idealized condition because virtually suggests that the spatial separation of atomic layers occurs uniformly over the whole surface of interaction of elements. The following approach to a more accurate description of the dynamics of crack growth is suggested. In this approach, it is assumed that breaking of the bond (linked \rightarrow unlinked transition of the state of the pair) is a time-space distributed process. This process is technically expressed through change of the dimensionless coefficient k_{link}^{ij} ($0 \leq k_{\text{link}}^{ij} \leq 1$). This coefficient has the meaning of the portion of linked part of the contact area S_{ij} . In this case the square of linked part of the contact area in

the pair $i-j$ is $S_{link}^{ij} = S_{ij} k_{link}^{ij}$, while $S_{unlink}^{ij} = S_{ij} (1 - k_{link}^{ij})$ is the square of unlinked part of this area. Thus, in this approach, the dynamics of bond breaking in a pair of elements is expressed by the dependence $k_{link}^{ij}(t)$, where k_{link}^{ij} decreases from initial value 1 (totally linked pair) to final value 0 (totally unlinked pair). Depending on the size of the discrete elements and features of the internal structure of fragment of the material, which is simulated by the discrete element (in particular, the presence of pores, damages, block structure) the stable or unstable crack growing model can be applied to describe the breakage of bond in the pair. These models are described in [6].

5 CONCLUSIONS

- An approach which makes possible fundamental extension of the application field of DE-based methods to elastic-plastic (as well as to visco-elastic-plastic) solids is proposed in the paper. This approach is based on the idea about building associations between the components of local stress/strain tensor and the inter-element forces/displacements. The proposed associating allows one to rewrite relations of the applied model of elasticity and plasticity (which are conventionally written in terms of stress/strain tensor components) in terms of forces and displacements or their increments.
- Another important advantage of the developed formalism of discrete element interaction is a possibility to directly apply complex multiparametric fracture criteria (Drucker-Prager, Mohr-Coulomb, etc) as criteria of interelement bond breakage. The use of these criteria is very important for correct modeling of fracture of complex heterogeneous materials of various nature. The method of calculation of these criteria for the pair of interacting elements is proposed in the paper.
- For correct modeling the processes of inelastic deformation and fracture of geological materials and media at "high" structural scales (relative to the scale of grains) the well-known Nikolaevsky's model of plasticity of rocks is implemented within the framework of mathematical formalism of discrete element method. The important features of this model are taking into account effect of pressure on the condition of reaching the yield state (beginning of inelastic deformation) and linear dependence of dilatation on plastic shear strain. Note that at present time this model as well as other analogous multiparametric dilatational models of plasticity are widely used within the formalism of conventional numerical methods of continuum mechanics (FEM, FDM and so on) to study mechanical processes in geomedium. Implementation of plasticity model of such kind within the framework of DEM is carried out for the first time.
- Developed mathematical formalism of DEM can be considered as the basis for building multiscale models of heterogeneous materials (including rocks) with hierarchically organized multiscale internal structure. Currently there are several approaches to the construction of such multiscale models. One of the approaches is developed by the authors of this paper and is called "integral" approach [10]. Under this approach, the parameters of applied rheological model of the material are considered as functions of the current values of local strains and strain rates (typically invariants of these tensors are used as arguments of functions). Main structural/spatial scales of lower ranks in relation to the considered one are defined.

For each distinct structural level, starting with the lowest, the so-called representative volume is determined. According to the results of theoretical study (analytical description or numerical DEM-based modeling) of the response of a representative volume the form of integral rheological dependence and the values of its parameters (including strength) are derived [2,10]. Thus constructed rheological models are then used as input data for the components of structure (regions with different structural phase composition) at a higher-level scale. The consistent implementation of this procedure, starting from the lowest selected scale up to macroscopic one, provides a macroscopic rheological model of brittle material. Being applied to non-associated plastic flow model of Nikolaevsky, the procedure of construction of multiscale model of rock (or geological medium) comes to determining the form and parameters of dependencies $Y(\epsilon_{ms}, \dot{\epsilon}_{ms})$, $\omega(\epsilon_{ms}, \dot{\epsilon}_{ms})$ and $\Lambda(\epsilon_{ms}, \dot{\epsilon}_{ms})$.

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